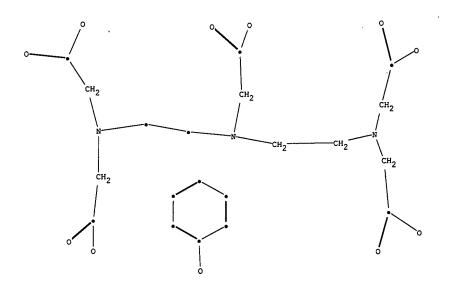
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     SCHMITTWIL, H; SCHUHMANNG, G; WEINMANN, H J; PLATZEK, H; PLAT-ZEK, J
PA
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     BERLIN & BERGKAMEN AG
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ANSWER 1 OF 12 CAPLUS COPYRIGHT 1997 ACS Document No. 126:80220 Molecular Mechanics Investigation 1996:653416 of Gadolinium(III) Complexes. Reichert, David E.; Hancock, Robert D.; Welch, Michael J. (Mallinckrodt Institute of Radiology, Washington University School of Medicine, St. Louis, NO, 63110, USA). Inorg. Chem., 35(24), 7013-7020 (English) 1996. CODEN: INOCAJ. ISSN: 0020-1669. OTHER SOURCES: CJACS-IMAGE; CJACS. AΒ Parameters for the com. available modeling package SYBYL have been developed for Gd3+ complexes allowing these to be studied with mol. mechanics. With these parameters and a technique termed the "coordination scan", the coordination nos. of Gd(III) based complexes can be predicted, and thus the hydration no. q detd. Knowledge of q has allowed the prediction of molar relaxivities based on correlations to literature values. In addn., the calcd. value .DELTA. Ecoord was found to successfully predict the thermodn. stability consts. for polyamino carboxylate ligands with Gd3+. Gadolinium complexes are commonly utilized as MRI contrast agents, and thus the techniques utilized in this work should aid in the

L3 ANSWER 2 OF 12 CAPLUS COPYRIGHT 1997 ACS

development of new contrast agents.

1996:605475 Document No. 125:230822 Diagnostic imaging contrast agents with extended blood retention. McMurry, Thomas J.; Sajiki, Hironao; Scott, Daniel M.; Lauffer, Randall B. (Metasyn, Inc., USA). PCT Int. Appl. WO 9623526 AZ 960808, 91 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE. (English). CODEN: PIXXD2.

APPLICATION: WO 96-US164 960116. PRIORITY: US 95-382317 950201. Scott, Daniel M.; Lauffer, Randall B. (Metasyn, Inc., USA). PCT AΒ Diagnostic imaging contrast agents which exhibit improved blood retention comprise: (a) an image-enhancing (or signal-generating) moiety (e.g. a heavy metal chelate); (b) a plasma protein-binding hydrophobic moiety; and (c) a blood half-life extending hydrophilic moiety (preferably a phosphate group). These contrast agents exhibit reduced rates of both renal and hepatocellular uptake and no apparent uptake by the reticuloendothelial system. The agents may be targeted to the blood pool or any other biol. component. Since the agent is lost less rapidly from the bloodstream, lower doses can be used at a higher margin of safety. Thus, MS-323 [Ph (CH2) 100P (O) (OH) OCH2CH [N (CH2CO2H) 2] CH2N (CH2CO2H) CH2CH2N (CH2CO2H) 2] Gd3+ complex (I) showed >95% binding to human serum albumin and a large area under the blood concn.-time curve. I was prepd. as the N-methylglucamine salt hydrate in 4 steps from 1-hydroxymethyl-DTPA penta-tert-Bu ester (prepd. from serine Me ester and ethylenediamine).

- L3 ANSWER 3 OF 12 APLUS COPYRIGHT 1997 ACS
 1996:462517 Docum No. 125:137213 Use of metal lexes as liver and gallbladder radiodiagnosis agents in computer tomography.

 Maier, Franz-Karl; Bauer, Michael; Krause, Werner; Speck, Ulrich; Schuhmann-Giampieri, Gabriele; Muehler, Andreas; Balzer, Thomas; Press, Wolf-Ruediger (Schering A.-G., Germany). PCT Int. Appl. WO 9616677 A2 960606, 118 pp. DESIGNATED STATES: W: AU, BY, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, SK, UA, VN; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 95-DE1644 951120. PRIORITY: US 94-351086 941130; US 95-387408 950213.
- Metal complexes consisting of a metal of at. no. 39-42, 44-51, or AB 56-83 and a complexing agent are used to produce x-ray contrast media for use in enhanced-contrast computed tomog. of the liver and bile ducts. The complexing agents are polyaminepolycarboxylic acids I [X = H, metal ion equiv.; x = 0-2; R1 = H, CR2R2L1(C6H4)mL2(C6H4)pL3R2; R2 = H, C1-6 aliph. chain; m, p = 0, 1;L1-L3 = single bond, O, S, NH, NR2, C1-10 alkylene, etc.; R3 = R1, or R3R3 = (substituted) (CH2)4; R4 = CHR1CO2X; if x = 2, R4 = CHR1CO2X or R4R4 = single bond]. Carboxyl groups which are not complexed may be present as salts of physiol. compatible cations or as amides of the form -C(O)NR12. Thus, the Gd(III) complex of 3, 6, 9-triaza-3, 6, 9-tris(carboxymethyl)-4-(4ethoxybenzyl)undecanedioic acid di-Na salt was administered i.v. at 0.2-0.5 mmol/kg to patients with liver metastases who were examd. 10, 60, and 120 min later by computed tomog. The scan d. of healthy liver tissue increased dose dependently, whereas that of the metastases remained unchanged. The gallbladder and bile ducts were also visualized.
- L3 ANSWER 4 OF 12 CAPLUS COPYRIGHT 1997 ACS
- 1996:462516 Document No. 125:137212 Use of chelate compounds as diagnostic agents in the x-ray examination of liver and bile ducts. Maier, Franz-Karl; Bauer, Michael; Krause, Werner; Speck, Ulrich; Schuhmann-Giampieri, Gabriele; Muehler, Andreas; Balzer, Thomas; Press, Wolf-Ruediger (Schering A.-G., Germany). PCT Int. Appl. WO 9616678 Al 960606, 5D pp. DESIGNATED STATES: W: AU, BY, CA, CN, CZ, F1, HU, JP, KR, MX, NO, NZ, PL, RU, SK, UA, VN; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 95-EP4547 951120. PRIORITY: US 94-351086 941130; US 95-387408 950213; US 95-480566 950607.
- AB Metal complexes of DTPA derivs. substituted with a benzyl group in the 4 or 5 position are suitable for use as contrast media in computed tomog. of the liver and the bile ducts. Suitable metals are of at. no. 44-51 and 56-83. Thus, the Gd(III) complex of 3,6,9-triaza-3,6,9-tris(carboxymethyl)-4-(4-ethoxybenzyl)undecanedioic acid di-Na salt was infused i.v. at 0.2-0.5 mmol/kg to patients with liver metastases who were examd. 10, 60, and 120 min later by computed tomog. The scan d. of healthy liver tissue increased dose dependently, whereas that of the metastases remained unchanged. The gallbladder and bile ducts were also visualized.
- L3 ANSWER 5 OF 12 CAPLUS COPYRIGHT 1997 ACS
- 1995:772691 Document No. 123:186924 Haloaryl-substituted metal complexes in a pharmaceutical medium, their use in diagnostics, and their preparation. Krause, Werner; Maier, Franz Karl; Press, Wolf-Ruediger; Schuhmann-Giampieri, Gabriele D.; Bauer, Michael; Schmitt-Willich, Heribert (Schering A.-G., Germany). Ger. Offen. DE 4341724 A1 950608, 36 pp. (German). CODEN: GWXXBX. APPLICATION: DE 93-4341724 931203.
- AB Polyaminopolycarboxylic acids and their transition metal, Group IIA, Group IIIA and Group IVA metal complexes, in particular Gd complexes were prepd. These complexes can be used in NMR and x-ray diagnostics.

- L3 ANSWER 6 OF 12 CAPLUS COPYRIGHT 1997 ACS
 1995:487801 Docum No. 122:240449 Preparation of matostatin analogs containing chelating groups and their radiolabeled compositions.. Albert, Rainer; Maecke, Helmut (Sandoz Ltd., Switz.; Sandoz-Patent-GmbH; Sandoz Erfindungen Verwaltungsgesellschaft M.B.H.). Eur. Pat. Appl. EP 607103 A2 940720 19 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 94-810008 940110. PRIORITY: GB 93-510 930112; GB 93-13129 930624; GB 93-15561 930728.
- AΒ XNHP [X = Q1, R1CH2R2NH; R21-R28 = H, alkyl, hydroxyalkyl; 1 of R29,R30 = H, alkyl, protecting group, the other = H, alkyl; s = 2-4; Z =divalent group; Y1 = bond, spacer group; R1 = bifunctional chelating group derived from a polyaminopolycarboxylic acid or anhydride bearing the moiety CH2R2NHY2 on a tertiary C atom; R2 = alkylene, (substituted) phenylene; Y2 = CO, spacer group having CO on one end and a CH2 group on the other, or having CO groups on both ends; PNH = N-terminal residue of a somatostatin], and salts and complexes with nuclides, were prepd. Thus, N,N,N',N'',N''-pentakis(tertbutoxycarbonylmethyl)-1-[(4-aminophenyl)methyl]diethylenetriamine was coupled to oxidized form Suc-D-Phe-Cys-Tyr-D-Trp-Lys(FMOC)-Thr-Cys-Thr-OH (Suc = succinyl) (prepn. given) using DCC/hydroxybenzotriazole in DMF followed by FMOC cleavage with piperidine in DMF and ester cleavage with CF3CO2H/ethanedithiol in CH2Cl2 to give title compd. I. The 111In complex of I was prepd. Title compds. are claimed for use as drugs and imaging agents.
- L3 ANSWER 7 OF 12 CAPLUS COPYRIGHT 1997 ACS
 1994:675494 Document No. 121:275494 Radiolabeled peptides, especially technetium-99m-labeled peptides, for diagnostic imaging. Dean, Richard T. (Diatech, Inc., USA). PCT Int. Appl. WO 9419024 A2
 940901, 35 pp. DESIGNATED STATES: W: AU, CA, JP, KR, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 94-US1894 940218. PRIORITY: US 93-19864 930219.
- This invention relates to reagents, radiolabeled reagents and methods for producing such reagents and radiolabeled reagents. Specifically, the invention relates to Tc-99m-labeled peptides that specifically bind to sites of infection, inflammation thrombosis, atherosclerosis and neoplastic growth in vivo, methods and kits for making such peptides, and methods for using such peptides to image sites in a mammalian body. Peptides were prepd. by solid phase peptide synthesis and radiolabeled with Tc-99m. Sites of infection in rabbits were imaged by scintigraphic imaging using Tc-99m-labeled Ackkkkc(Acm)GGPLYKKIIKKLLES (Acm = acetamidomethyl).
- L3 ANSWER 8 OF 12 CAPLUS COPYRIGHT 1997 ACS
 1992:194874 Document No. 116:194874 Preparation of
 diethylenetriaminetetraacetic acid complexes as contrast agents as
 diagnostic agents.. Schmitt-Willich, Neribert; Platzek, Johannes;
 Gries, Heinz; Schuhmann-Giampieri, Gabriele; Vogler, Hubert;
 Weinmann, Hanns Joachim (Schering A.-G., Germany). Eur. Pat. Appl.
 EP 405704 A2 910102, 26 pp. DESIGNATED STATES: R: AT, BE, CH, DE,
 DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (German). CODEN: EPXXDW.
 APPLICATION: EP 90-250165 900627. PRIORITY: DE 89-3922005 890630.

 AB Title compds. [I; Z1, Z2 = H, (CH2)m-(C6H4)q-Ok-(CH2)n-(C6H4)T-Or-R;
 m. n = 0. 1-20 integer: k, l, g, r = 0. 1: R = H (substituted)
- m, n = 0, 1-20 integer; k, 1, q, r = 0, 1; R = H, (substituted) alkyl, CH2CO2R1; R1 = H, alkyl, benzyl; X = H, metal ion, etc.; other provisos] were prepd. 3,6,9-Triaza-3,6,9-tris(tert-butoxycarbonylmethyl)-4-(4-hydroxybenzyl)undecandicarboxylic acid di-tert-Bu ester was O-methylated with MeI in THF contg. NaH to give the 4-methoxybenzyl deriv., which was hydrolyzed and then reacted with Gd2O3 in water to give I [Z1 = 4-methoxybenzyl; Z2 = X = H] Gd complex (II). II at 0.06 mmol/kg i.v. gave very clear nuclear spin tomograms of rat organs compared with the control.

ANSWER 9 OF 12 APLUS COPYRIGHT 1997 ACS 40918 Docume No. 116:40918 Preparation No. 116:40918 Preparation of A monoamides and 1992:40918 their metal complexes as contrast agents for NMR imaging. Gries, Heinz; Klieger, Erich; Raduechel, Bernd; Schmitt-Willich, Heribert; Weinmann, Hanns Joachim; Vogler, Hubet; Schuhmann-Giampieri, Gabriele; Conrad, Juergen (Schering A.-G., Germany). Eur. Pat. Appl. EP 450742 A1 911009, 25 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE. (German). CODEN: EPXXDW. APPLICATION: EP 91-250089 910405. PRIORITY: DE 90-4011684 900406.

Title compds. (XO2CCH2)2NCHZ1CHZ2N(CH2CO2X)(CH2)2N(CH2CO2X)CH2CONR2R AΒ 3 [Z1, Z2 = H, (CH2)m(C6H4)q(O)k(CH2)n(C6H4)1(O)rR; m, n = 0-20; k, 1, q, 4r = 0, 1; R = H, (substituted) C1-6 alkyl, CH2CO2R1; R1 = H, C1-6 alkyl, CH2Ph; R2, R3 = aryl, aralkyl, carboxy- or sulfonyl-substituted C1-20 (cyclic) alkyl, etc.; X = H, metal ion of at. no. 21-29, 31, 32, 37-40, 42-44, 49, 57-83; with provisos] were prepd. as contrast agents for NMR imaging. Thus, N3-(2,6-dioxomorpholinoethyl)-N6-(ethoxycarbonylmethyl)-3.6diazaoctanedicarboxylic acid (prepn. given) in DMF was treated with Et3N and 11-aminoundecanoic acid and the resulting product hydrolyzed to give 3,6-bis(carboxymethyl)-9-(10carboxydecylcarbamoylmethyl)-3,6.9-triazaundecanedicarboxylic acid The complex formed from 15 mmol I and 7.5 mmol Gd203 was prepd. and used as a contrast agent for NMR imaging.

ANSWER 10 OF 12 CAPLUS COPYRIGHT 1997 ACS L3Document No. 112:140769 Polymer-bonded complexing agents 1990:140769 and their complexes for use in pharmaceuticals. Deutsch, Julius; Schmitt-Willich, Heribert; Gries, Heinz; Conrad, Juergen; Neumeier, Reinhard (Schering A.-G., Fed. Rep. Ger.). Ger. Offen. DE 3806795

(German). CODEN: GWXXBX. APPLICATION: DE A1 890907, 47 pp.

88-3806795 880229.

The title complexing agents, useful in diagnosis and therapy, consists of polymers bearing CO2H or P acid groups and, optionally, ions with at. no. 21-29, 31, 32, 37-39, 42-44, 49, or 57-83 or cations of inorg. or org. bases, amino acids, or amino amides. Stirring 7.6 g di-tert-Bu 2,6,9-tris[(tert-butoxycarbonyl)methyl]-4-(4-carbomethoxybenzyl)undecanedioate (the multistep prepn. of which is described), 1.28 g iso-Bu chloroformate, 1.9 g Et3N, and 100 mL THF at 0.degree. for 1 h, adding an aq. soln. of 533.2 mg polyethylenimine with cooling, and stirring at room temp. gave 4.35 g cryst. powder which formed a Gd complex contg. 20.67% Gd. Similar Gd complexes were used as contrast agents in the diagnosis of tumors by NMR.

ANSWER 11 OF 12 CAPLUS COPYRIGHT 1997 ACS Document No. 112:135602 Cyclic aliphatic aza complexants, 1990:135602 complexes and complex salts, process for their preparation and pharmaceutical agents containing them. Deutsch, Julius; Conrad, Juergen (Schering A.-G., Fed. Rep. Ger.). Eur. Pat. Appl. EP 305320

A2 890301, 37 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE. (German). CODEN: EPXXDW. APPLICATION:

EP 88-730187 880823. PRIORITY: DE 87-3728525 870824.

The aliph. aza derivs. I and II [B, D, E = (CH2)k(CHR2)n(CH2)1; R, R1, R2 = H, (un) substituted alkylene having terminal functional group or macromol.; V = Q, radical related to I or II; A =(CH2) mCHR2 (CH2)1; V1 = V, CH2X; X = CO2Y, PO3HY; Y = H, metal; k, 1 = 0-5; m = 1-5; n = 0, 1; q = 0-2; r = 0-3] are prepd. as complexing agents and complexes for diagnosis and therapy (no data). A soln. of 3-aza-1-(4-hydroxybenzyl)-N,N,N,N-pentakis-(8-aza-2-hydroxy-4oxa-6,10-diaminodecyl)pentane-1,5-diamine (prepn. given) and Et3N in MeOH was treated with a soln. of di-tert-Bu 3,6,9-triaza-3,6,9tris(tert-butoxycarbonylmethyl)-4-[(oxiranylmethoxy)methyl]undecaned icarboxylate in MeOH, followed by refluxing for 36 h, to give 3-aza-1,5-diamino-2-(4-hydroxybenzyl)-N,N,N,N-pentakis[8-aza-6,10diamino-2-hydroxy-4-oxa-N', N', N', N', n'-pentakis-2-hydroxy-4-oxa-6, 10-

bis[di(carboxymethylamino)]-8-(carboxymethylaza) cyldecyl]pentane, d into Gd complexes. which was conv

ANSWER 12 OF 12 CAPLUS COPYRIGHT 1997 ACS 1989:554376 Document No. 111:154376 Preparation of (carboxymethylamino)ethylene oligomers and their metal complexes for use as nuclear magnetic resonance and radiographic imaging agents. Deutsch, Julius; Gries, Heinz; Klieger, Erich; Niedballa, Ulrich; Renneke, Franz Josef; Conrad, Juergen; Muetzel, Wolfgang (Schering A.-G., Fed. Rep. Ger.). Ger. Offen. DE 3710730 A1 881020, 57 pp. (German). CODEN: GWXXBX. APPLICATION: DE 87-3710730 870331. The title compds. [I; R1, R2 = H, (substituted) (imino-, phenyleneoxy-, O-, S-, etc. contg.) C1-20 alkylene terminated by another I moiety (connected at R1 or R2) or by a macromol.; X = H, metal ion selected from elements with at. nos. 21-29, 31, 32, 38, 39, 42-44, 49, 57-83; m, n = 0-4, m + n .ltoreq.4], useful as diagnostic imaging agents, for radiotherapy, and as haptens for prepn. of antibodies (no data) were prepd. 4-HOC6H4CH2CH(NH2)CH2NH2.2HCl in DMF contg. KHCO3 was treated at 35.degree. with BrCH2CO2CMe3 in DMF and the mixt. was stirred 2-5 h to give 63% Me3CO2CCH2NHCH(CH2C6H4OH-4)CH2NHCH2CO2CMe3. The latter in THF was treated with NaH and then PhCH2O2CNH(CH2)3Br in THF. mixt. was stirred overnight and the product was hydrogenolyzed, condensed with maleic anhydride, and hydrolyzed with CF3CO2H to give 3,6-diaza-3,6-bis(carboxymethyl)-4-[4-(3-

maleimidopropoxy)benzyl]suberic acid. The Gd complex of the latter

was prepd. in NH4OAc-ag using Gd(OAc)3.

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     DTPA-mono amide derivs. useful in diagnostics and radiotherapy -
     especially as NMR contrast agents, e.g. for pinpointing tumours in
     the hepatobiliary and gastrointestinal system.
DC
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     CONRAD, J; GRIES, H; KLIEGER, D E; RADUCHEL, B; SCHMITT-WILLICH, H;
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     SCHUHMANN-GIAMPIERI, G; VOGLER, H; WEINMANN, H; KLIEGER, E; SCHMITT,
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